Poly(ether ether ketone) (PEEK) XPS reference core level and energy loss spectra

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Poly(ether ether ketone) (PEEK) XPS Reference Core Level and Energy Loss Spectra

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XPS measurements of poly(ether ether ketone) recorded with a SSX-100 spectrometer in standardized experimental conditions are presented: survey scan, high resolution core level spectra as well as the energy loss regions of carbon and oxygen peaks are analyzed. This is part of a contract work aiming to record spectra in the very same conditions of some 40 different polymers. © *2006 American Vacuum Society.* [DOI: 10.1116/11.20051106]

Keywords: *x-ray photoelectron spectroscopy; XPS; surface; polymer; poly(ether ether ketone); PEEK*

PACS: *79.60.Fr, 82.80.Pv, 79.20.Uv, 61.41.+e, 01.30.Kj*

Accession # 00891
Technique: XPS
Host Material: poly(ether ether ketone)
Instrument: Surface Science Instruments SSX-100
Major Elements in Spectrum: C, O
Minor Elements in Spectrum: none
Printed Spectra: 5
Spectra in Electronic Record: 5
Spectral Category: comparison

SPECIMEN DESCRIPTION

Host Material: poly(ether ether ketone)

CAS Registry #: 31694-16-3

Host Material Characteristics: homogeneous; solid; amorphous; dielectric; polymer

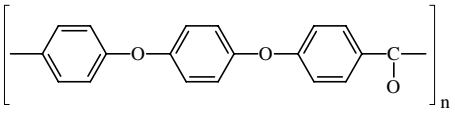
Chemical Name: poly(ether ether ketone)

Source: ICI

Host Composition: not specified

Form: pellet

Structure:



History & Significance: This study is a part of a reference spectra database of polymers, including survey and core level spectra, but also energy loss spectra of the main elements.

As Received Condition: not specified

Analyzed Region: same as host material

***Ex Situ* Preparation/Mounting:** pressed powder

***In Situ* Preparation:** none

Pre-Analysis Beam Exposure: The analyzed region was exposed to x-rays for a very short time, around 2 min for sample position adjustment prior to measurements.

Charge Control: use of a metal screen and a flood gun (2 eV)

Temp. During Analysis: 300 K

Pressure During Analysis: $<6.6\times10^{-8}$ Pa

INSTRUMENT DESCRIPTION

Manufacturer and Model: Surface Science Instruments SSX-100

Analyzer Type: spherical sector

Detector: position sensitive detector with microchannel plate

Number of Detector Elements: 128

INSTRUMENT PARAMETERS COMMON TO ALL SPECTRA

■ *Spectrometer*

Analyzer Mode: constant pass energy

Throughput ($T=E^N$): N=See comment below

Throughput Comment: $T = E^N$, $N = 0.7$

Excitation Source Window: 1.5 μm Al foil

Excitation Source: Al K_α monochromatic

Source Energy: 1486.6 eV

Source Strength: 130 W

Source Beam Size: 0.6 mm × 0.6 mm

Signal Mode: not specified

■ *Geometry*

Incident Angle: 57.6°

Source to Analyzer Angle: 70.8°

Emission Angle: 14.7°

Specimen Azimuthal Angle: 75.5°

Acceptance Angle from Analyzer Axis: 0°

Analyzer Angular Acceptance Width: 30° × 30°

DATA ANALYSIS METHOD

Energy Scale Correction: To compensate for charging effects, we adjusted the largest C 1s component to 284.70 eV (Ref. 1).

Recommended Energy-Scale Shift: +6.03 eV

Peak Shape and Background Method: A least square fitting routine with mixed Gaussian/Lorentzian for the components and a linear background was used.

Quantitation Method: Scofield factors corrected for energy dependence were used.

ACKNOWLEDGMENTS

This study is a part of the EU-BCR contract ''XPS Spectral Intensity Data Bank.'' We thank the NPL for authorizing us to publish these spectra.

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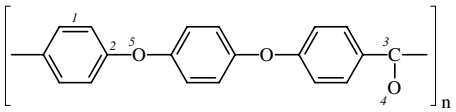
REFERENCES

1. G. Beamson and D. Briggs, in *The Scienta ESCA 300 Database* (Wiley, Chichester, 1992).
2. C. J. Powell, J. Electron. Spectrosc. Relat. Phenom. **47**, 197 (1988).

SPECTRAL FEATURES TABLE

Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV-cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
00891-02	C 1*s*	284.70	1.11	7815	1.00	64.5	1 in Diagram below
00891-02	C 1*s*	286.31	1.09	1915	1.00	16.0	2 in Diagram below
00891-02	C 1*s*	287.10	0.94	213	1.00	1.8	3 in Diagram below
00891-02	C 1*s*	291.59	1.81	405	1.00	⋯	⋯
00891-03	O 1*s*	531.31	1.42	1445	2.49	4.9	4 in Diagram below
00891-03	O 1*s*	533.40	1.30	3542	2.49	11.9	5 in Diagram below
00891-03	O 1*s*	540.91	3.29	154	2.49	⋯	⋯

Comment to Spectral Features Table:



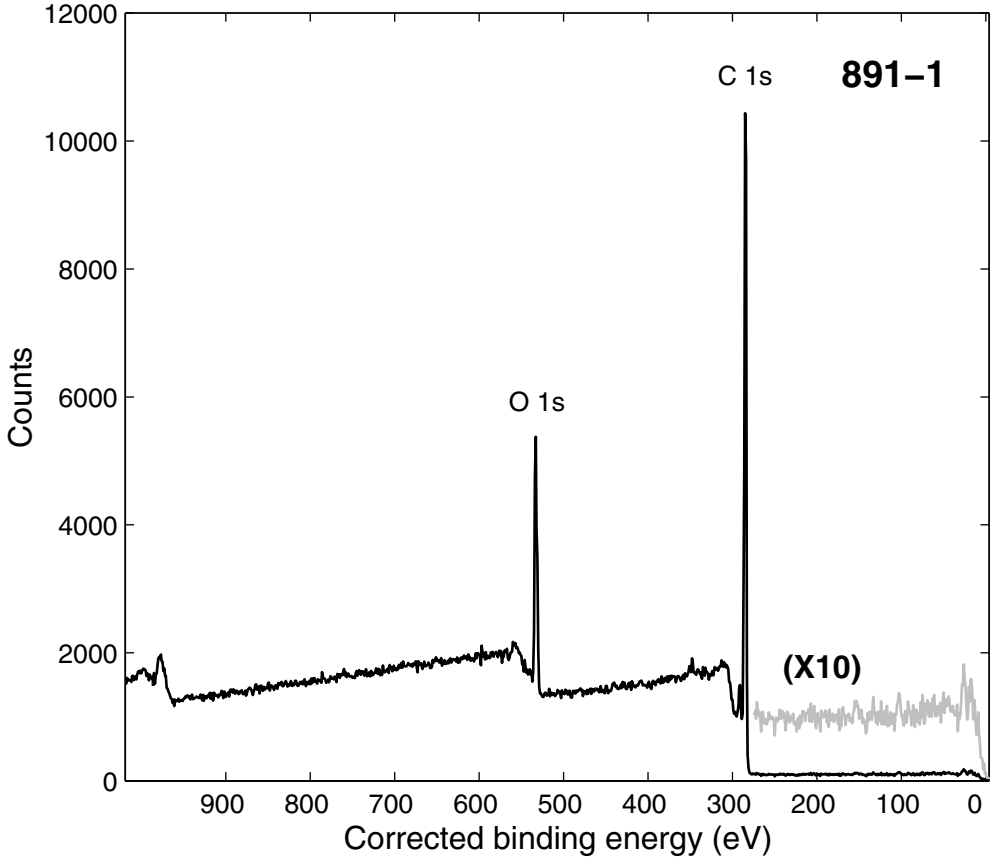
ANALYZER CALIBRATION TABLE

Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV-cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
⋯	Cu $2p_{3/2}$	932.34	1.19	202906	9.748	⋯	⋯
⋯	Cu $3p_{3/2}$	74.78	2.36	289045	2.774	⋯	⋯

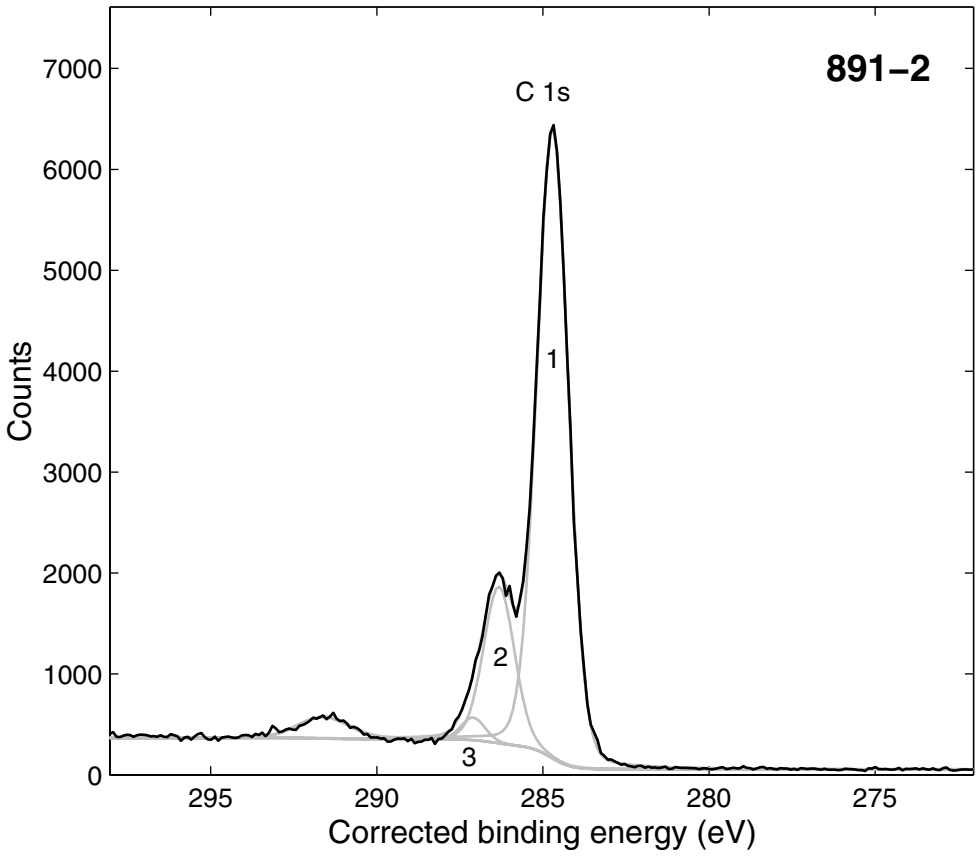
GUIDE TO FIGURES

Spectrum (Accession) #	Spectral Region	Voltage Shift*	Multiplier	Baseline	Comment #
891-1	Survey	−6.03	1	0	
891-2	C 1*s*	−6.03	1	0	
891-3	O 1*s*	−6.03	1	0	
891-4	C 1*s* + losses	−6.03	1	0	
891-5	O 1*s* + losses	−6.03	1	0	

* Voltage shift of the archived (as-measured) spectrum relative to the printed figure. The figure reflects the recommended energy scale correction due to a calibration correction, sample charging, flood gun, or other phenomenon.

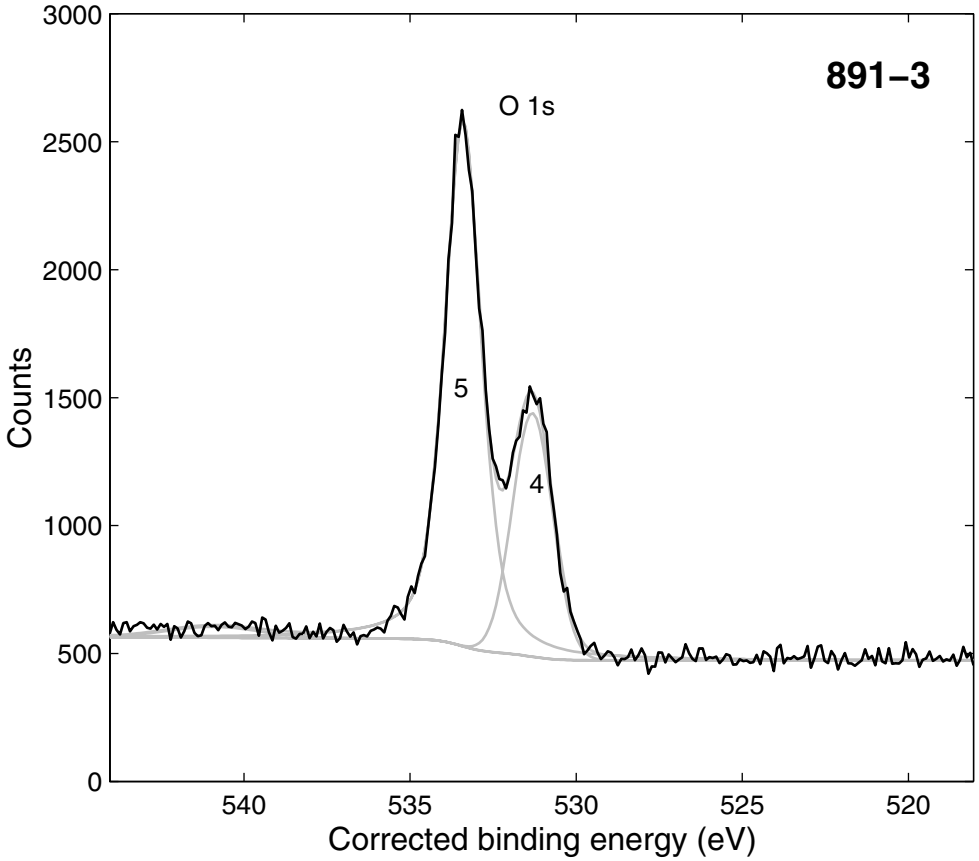


Accession #	00891-01
Host Material	poly(ether ether ketone)
Technique	XPS
Spectral Region	survey
Instrument	Surface Science Instruments SSX-100
Excitation Source	Al K_α monochromatic
Source Energy	1486.6 eV
Source Strength	130 W
Source Size	0.6 mm × 0.6 mm
Analyzer Type	spherical sector
Incident Angle	57.6°
Emission Angle	14.7°
Analyzer Pass Energy	106.8 eV
Analyzer Resolution	1.17 eV
Total Signal Accumulation Time	960 s
Total Elapsed Time	not specified
Number of Scans	2
Effective Detector Width	12.96 eV



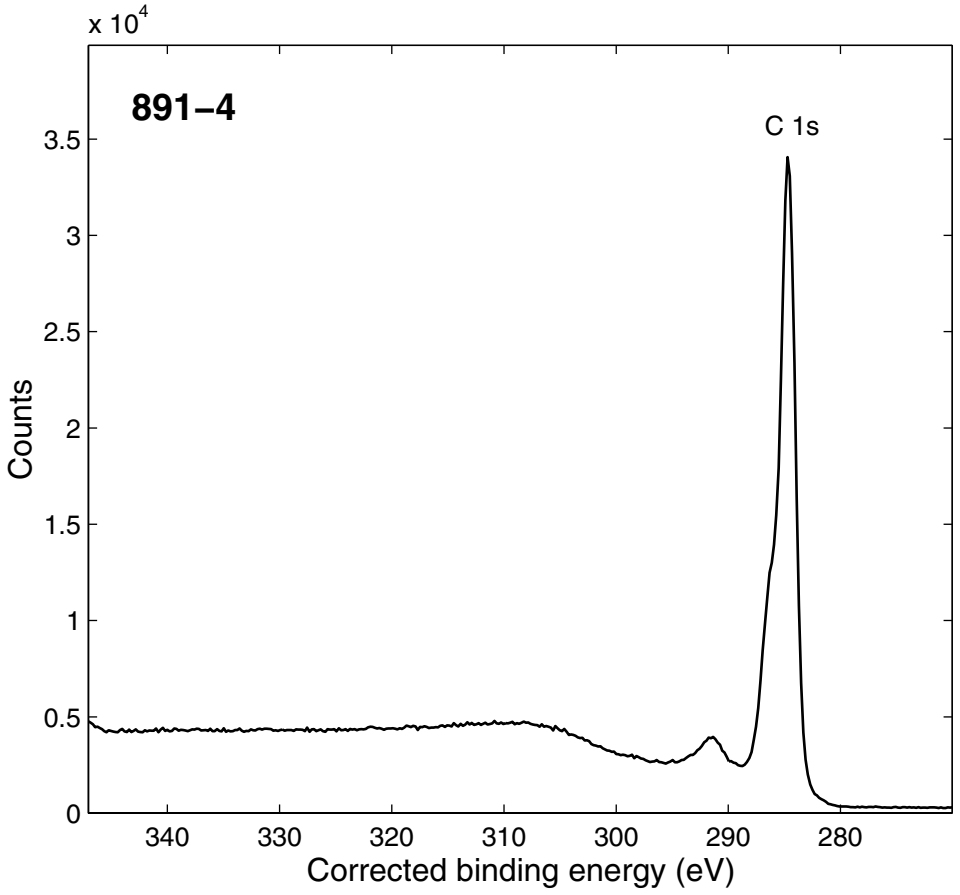
- **Accession #:** 00891-02
- **Host Material:** poly(ether ether ketone)
- **Technique:** XPS
- **Spectral Region:** C 1*s*

Instrument: Surface Science Instruments SSX-100
Excitation Source: Al K_α monochromatic
Source Energy: 1486.6 eV
Source Strength: 130 W
Source Size: 0.6 mm × 0.6 mm
Incident Angle: 57.6°
Analyzer Type: spherical sector
Analyzer Pass Energy: 29.97 eV
Analyzer Resolution: 0.76 eV
Emission Angle: 14.7°
Total Signal Accumulation Time: 1200 s
Total Elapsed Time: not specified
Number of Scans: 10
Effective Detector Width: 3.341 eV



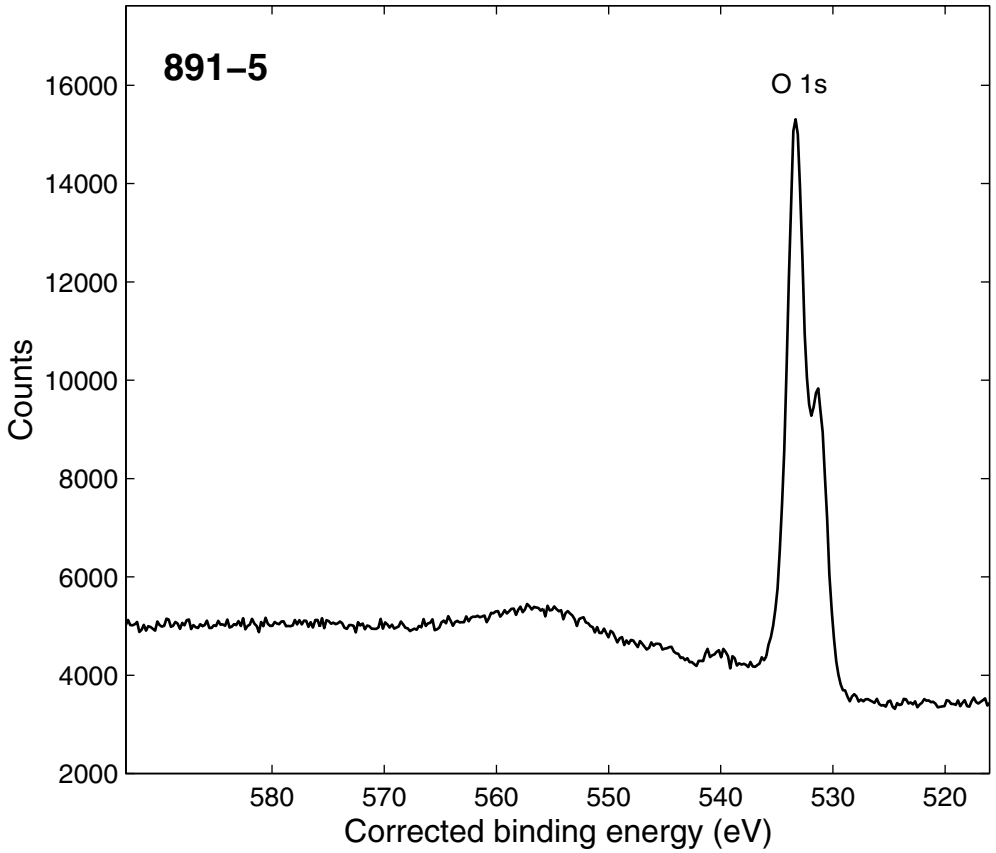
- **Accession #:** 00891-03
- **Host Material:** poly(ether ether ketone)
- **Technique:** XPS
- **Spectral Region:** O 1*s*

Instrument: Surface Science Instruments SSX-100
Excitation Source: Al K_α monochromatic
Source Energy: 1486.6 eV
Source Strength: 130 W
Source Size: 0.6 mm × 0.6 mm
Incident Angle: 57.6°
Analyzer Type: spherical sector
Analyzer Pass Energy: 29.97 eV
Analyzer Resolution: 0.76 eV
Emission Angle: 14.7°
Total Signal Accumulation Time: 1200 s
Total Elapsed Time: not specified
Number of Scans: 10
Effective Detector Width: 3.341 eV



- **Accession #:** 00891-04
- **Host Material:** poly(ether ether ketone)
- **Technique:** XPS
- **Spectral Region:** C 1*s* energy losses

Instrument: Surface Science Instruments SSX-100
Excitation Source: Al K_α monochromatic
Source Energy: 1486.6 eV
Source Strength: 130 W
Source Size: 0.6 mm × 0.6 mm
Incident Angle: 57.6°
Analyzer Type: spherical sector
Analyzer Pass Energy: 106.8 eV
Analyzer Resolution: 1.17 eV
Emission Angle: 14.7°
Total Signal Accumulation Time: 900 s
Total Elapsed Time: not specified
Number of Scans: 5
Effective Detector Width: 12.956 eV



- **Accession #:** 00891-05
- **Host Material:** poly(ether ether ketone)
- **Technique:** XPS
- **Spectral Region:** O 1*s* energy losses

Instrument: Surface Science Instruments SSX-100
Excitation Source: Al K_α monochromatic
Source Energy: 1486.6 eV
Source Strength: 130 W
Source Size: 0.6 mm × 0.6 mm
Incident Angle: 57.6°
Analyzer Type: spherical sector
Analyzer Pass Energy: 106.8 eV
Analyzer Resolution: 1.17 eV
Emission Angle: 14.7°
Total Signal Accumulation Time: 900 s
Total Elapsed Time: not specified
Number of Scans: 5
Effective Detector Width: 12.956 eV